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Scientific Paper No. 30

Orthogonal Polynomials as a Basis for Objective Analysis

by R. DIXON, B.Sc.

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SUMMARY

The present computer analysis of meteorological fields by grid-pointwise techniques, in which the analytical process is repeated at every one of a large number of grid points, is described and certain limitations are mentioned. An alternative approach is presented in which a high-power bivariate polynomial is fitted to the data over a large area; the results for several such areas are joined together to form the complete analysis. Orthogonal polynomials are used to overcome computational difficulties in the fitting of high-powered polynomials. Examples of some preliminary results obtained by this new technique are presented in appendices.

INTRODUCTION

The numerical forecasting process at present in use in the Meteorological Office requires as its starting point a field of pressure-height values at the grid points of a rectangular area. The observations of pressure height are made at stations which are irregularly distributed within this area and consequently the problem arises of finding the rectangular grid-point values from this irregular geographical distribution. Bearing in mind that the observations incorporate various types of error, the analysis is obviously a complicated problem in interpolation. In the search for a solution to this problem the principle of least squares is used for the fitting technique.

The traditional method of solving the least-squares problem is to set up the system of 'normal equations' and solve them for the unknown coefficients in the fitting expression, and this is what is done in the analysis system currently used by the Meteorological Office. Whilst this approach is theoretically straightforward, in practice it is subject to certain limitations, a principal difficulty being the marked tendency of the normal equations to be ill-conditioned for anything other than low-powered fitting expressions. This restriction to low-powered polynomials means in turn that it is necessary to deal with the analysis grid point by grid point, since low-powered polynomials are not capable of describing the variations over the area covered by a large number of grid points. The result is a relatively rough analysis, having zero-order discontinuities between each point, which has been expensively obtained in terms of computer time because the procedure has had to be repeated at each grid point. Besides these present drawbacks there is the consideration that data from the sophisticated technology of the seventies will require analysis in four dimensions. An extension of the present cumbersome system to four dimensions scarcely seems reasonable.

An alternative approach to the problem is to use orthogonal polynomials in the fitting technique. When this is done the normal equations reduce to a set of independent equations each yielding one of the unknown coefficients, the problem of ill-conditioning is greatly reduced and polynomial expressions of high power having a great number of degrees of freedom can be used, enabling an area covered by a large number of grid points to be analysed at one time.

It is the purpose of this paper to give an outline of the orthogonal technique and to present some preliminary results which indicate the possibility of obtaining acceptably accurate and

speedy analyses by some analysis system utilizing this principle. Although comparisons are made at various places in the paper between the orthogonal technique and the traditional one this is done primarily to facilitate understanding of the orthogonal process. It is not the purpose of the paper to criticize any particular analysis system being used at present.

THE TRADITIONAL LEAST-SQUARES APPROACH

If matrix notation is used, a set of linear equations may be written

$$\mathbf{z} = \Phi\mathbf{a} \qquad \ldots (1)$$

where $\mathbf{a}$ is the vector of unknowns and Φ is the matrix of coefficients.

If the number of equations is equal to the number of unknowns then the solution to (1) is given by

$$\mathbf{a} = \Phi^{-1}\mathbf{z} \qquad \ldots (2)$$

On the other hand, if the number of equations is greater than the number of unknowns then it may be shown that the least-squares solution to (1) is given by the solution of the normal equations

$$\tilde{\Phi}\Phi\mathbf{a} = \Phi\mathbf{z} \qquad \ldots (3)$$

where $\tilde{\Phi}$ is the transpose of Φ.

The meteorological analysis problem is concerned with this latter situation. To be specific, an attempt is made to approximate the field of observations within a small area of the chart by fitting, for example, a quadric surface of best fit, in the least-squares sense, to these observations. This means that in the quadric

$$z = a_0 + a_1x + a_2y + a_3x^2 + a_4xy + a_5y^2 \qquad \ldots (4)$$

the particular values of the coefficients $a_0, a_1, \ldots, a_5$ which give this best fit are determined. These are the values given by (3). The derivation of the normal equations is given by Brooks and Carruthers,[1]* and a review of techniques for solving them is given in the first two chapters of *Modern computing methods.*[2]

The size of the array $\tilde{\Phi}\Phi$ depends solely on the number of terms in the expression to be fitted. Thus a third-power bivariate expression will have 10 terms in it and will lead to a 10×10 array for the matrix $\tilde{\Phi}\Phi$. This rapid growth in the size of the array is unfortunate as it means that the computational procedure for its solution becomes extremely cumbersome and time consuming, even for a digital computer. A further and more serious difficulty is that for large arrays the problem of ill-conditioning of the matrix $\tilde{\Phi}\Phi$ (see Berztiss[3] and Forsythe[4]) is encountered; this arises from the fact that for a more or less evenly distributed set of observations the determinant of $\tilde{\Phi}\Phi$ approximates to a principal minor of the infinite Hilbert determinant.[5] The Hilbert determinant of order n has the value

$$H_n = \frac{[1!\,2!\,3!\,\ldots\,(n-1)!]^3}{n!\,(n+1)!\,\ldots\,(2n-1)!} \qquad \ldots (5)$$

and this approaches zero rapidly as n increases. For example, when $n=2$, H_n is $8{\cdot}3 \times 10^{-2}$, but for $n=6$, $H_n = 5{\cdot}4 \times 10^{-18}$. Since the determinant of $\tilde{\Phi}\Phi$ figures in the denominator of the solution of equation (3) for $\mathbf{a}$, the estimates for the individual values a_r become unreliable. Some examples of ill-conditioning are given by Stephenson[6] and Bickley and Thompson.[7]

* The superscript figures refer to the bibliography on page 12.

The implications of this phenomenon with respect to the meteorological analysis problem are obvious. In current Meteorological Office practice the observation area is piecewise fitted by quadric surfaces and a 6×6 array is partly solved, and it is certain that the condition of the array is sometimes not good. The Meteorological Office has a unique position in the numerical engineering field in that it needs to know the answers to the nearest 5 metres only, and this reduces the problem. It is significant however, that when an attempt was made to improve upon the analysis quality by using cubic surfaces this failed, it being reported[8] that the use of cubics brought about no improvement. At least part of the reason may have been that the use of a 10×10 array brought about a worsening of the condition of the array.

The inevitability of this difficulty and the cumbersome nature of the computations are severe limitations on the traditional method. It represents a kind of strait-jacket, limiting the field of application of the method to such problems as can be dealt with by a low-power fitting. In the current Office practice these limitations are accepted and the regular grid of approximated values are obtained one at a time by fitting a quadric surface to a small area around each grid point, the grid point being taken as a local origin.[8] The constant term in the quadric expression then provides the fitted height. The restriction to a quadric fitting means that the grid points must necessarily be calculated one at a time, because the 6 coefficients of a quadric expression do not provide enough degrees of freedom to account for the sort of variation which a meteorological pressure surface can have in practice over any substantial area. Indeed even for a small area around the grid point the degrees of freedom are often inadequate, resulting in a poor fit on occasions when an intense feature is present, and it has been found necessary to introduce additional computational devices to compensate for this.

Acceptance of this basic limitation has certain disadvantages. If the present grid is used, carrying out the pivotal condensation procedure plus subsidiary routines at each grid point requires the repetition of the process 1927 times for each level analysed. In the end, because there is no simple functional relationship connecting each grid-point height to the next one, the analysis obtained is rough, in the sense that there are discernible zero-order discontinuities between each grid point. Whilst the zero-order fields are just about acceptable, the roughness in the higher-order fields is intolerable, and for various purposes time has to be spent smoothing them.

There is the additional disadvantage that since only the constant is required this is the only term that is calculated, with the result that there is in fact no reference surface actually computed against which to judge the correctness of the original observations. This necessitates a second sweep in which planes are fitted to each group of four grid points. Observations are then rejected if they lie more than a certain distance off these planes.

Looking ahead to future requirements the limitation on the traditional method is even more oppressive. To meet the requirements of a multilayered forecast model it will be desirable to be able to achieve a rigorous least-squares fitting of observations throughout a substantial volume of space, i.e. it must be possible to fit in three dimensions without recourse to the inadequate expedients of pointwise fitting or of fitting independently at different levels and then trying to adjust through columns. An interesting attack on the problem by means of a columnwise extension of the current grid-pointwise practice was made by Corby.[9]

The severity of the three-dimensional fitting problem will be realized on contemplating the trivariate second-power expression

$$v = a_0 + a_1x + a_2y + a_3z + a_4x^2 + a_5xy + a_6y^2 + a_7zx + a_8zy + a_9z^2. \quad \ldots (6)$$

This has 10 terms and to achieve a fitting with it means solving a 10×10 array. This means that even to achieve a second-power fitting, which would be appropriate only to the observations within a small volume of space, the computations are well into the region where ill-conditioning may occur, and even a grid-pointwise fitting, analogous to the present technique at one level, might well prove inadequate. The difficulty of achieving anything more sophisticated is instantly apparent in Table I.

TABLE I. *Number of terms in a trivariate polynomial*

Power (p)	No. of terms (n)
1	4
2	10
3	20
4	34
5	56
6	84

The general term is in fact

$$n = \frac{(p+1)(p+2)(p+3)}{3!}. \qquad \ldots (7)$$

The three-dimensional problem is not the only one facing the Meteorological Office. In a sense the four-dimensional problem already exists, for there is a wealth of high-class observational material to hand from modern aircraft flying the globe. Radar heights and Doppler winds provide excellent analysis material, but the heights and winds are typically for times other than the main synoptic hours and for levels other than the standard pressure-levels, and hence set a difficult problem. There is also the prospect of merchant ships sending up sondes at non-standard times. The hopelessness of accommodating this material by means of the traditional technique is quite apparent if, say, the second-power quadrivariate expression (8) and Table II, as follow, are considered:

$$\begin{aligned} v = {} & a_0 + a_1 x + a_2 y + a_3 z + a_4 t \\ & + a_5 x^2 + a_6 yx + a_7 y^2 + a_8 zx + a_9 zy + a_{10} z^2 \\ & + a_{11} xt + a_{12} yt + a_{13} zt + a_{14} t^2. \end{aligned} \qquad \ldots (8)$$

TABLE II. *Number of terms in a quadrivariate polynomial*

Power (p)	No. of terms (n)
1	5
2	15
3	35
4	70
5	126
6	210

The general term is

$$n = \frac{(p+1)(p+2)(p+3)(p+4)}{4!}. \qquad \ldots (9)$$

It is clear that as long as the traditional method is used, ill-conditioning and the general cumbersome nature of the method will prevent anything other than an elementary and unsatisfactory use of such material. Furthermore, the present grid-pointwise approach does not lend itself to the development of the sort of sophisticated quality control and intervention procedures which should be the natural concomitants of an advanced analysis process, neither does it provide for the sort of versatility desirable in future output routines. For example, a requirement for an analysis for a non-standard level for a non-standard time would be difficult to meet at present and the result would be unsatisfactory when obtained. As another instance, a future analysis procedure should be capable of providing the forecaster not merely with an analysis for a level but also with a properly constituted vertical cross-section along any line. Such refinements will however be extremely difficult to provide as long as grid-pointwise methods are the only ones available.

The way out of this impasse is to resort to an orthogonal approach.

THE ORTHOGONAL LEAST-SQUARES METHOD

To make this method clear it is desirable to introduce the concept of function space, a full account of which is to be found in Synge.[10]

Consider a set of observations of pressure height $h_0, h_1, \ldots, h_n$ where these heights are listed in any order; the set can be represented as a vector as follows.

$$\mathbf{h} = \mathrm{h}_0\mathbf{i}_0 + \mathrm{h}_1\mathbf{i}_1 + \mathrm{h}_2\mathbf{i}_2 + \ldots + \mathrm{h}_n\mathbf{i}_n \qquad \ldots (10)$$

where $\mathbf{i}_0, \mathbf{i}_1, \ldots, \mathbf{i}_n$ are rectilinear unit vectors. Now, instead of fitting the expression

$$z = a_0 + a_1x + a_2y + a_3x^2 + a_4xy + a_5y^2, \qquad \ldots (4)$$

fit instead the expression

$$z = a_0\phi_0 + a_1\phi_1 + a_2\phi_2 + a_3\phi_3 + a_4\phi_4 + a_5\phi_5 \qquad \ldots (11)$$

where the ϕs are themselves polynomials in the variables x and y and to the same order as in the corresponding term of (4). That is to say

$$\left.\begin{aligned}
\phi_0 &= b_0 \\
\phi_1 &= c_0 + c_1x \\
\phi_2 &= d_0 + d_1x + d_2y \\
\phi_3 &= e_0 + e_1x + e_2y + e_3x^2 \\
\phi_4 &= f_0 + f_1x + f_2y + f_3x^2 + f_4xy \\
\phi_5 &= g_0 + g_1x + g_2y + g_3x^2 + g_4xy + g_5y^2.
\end{aligned}\right\} \qquad \ldots (12)$$

Equation (11) is simply a more general form of (4), and in writing (11) instead of (4) all the coefficients in the equations of (12) become available. As will be seen later the coefficients in (12) can be chosen to give the ϕs a remarkable property.

Consistent with the expression of the observed heights as a vector, the evaluations of each ϕ polynomial over the field of x, y values can be regarded as the components of a $\boldsymbol{\phi}$ vector. Thus, for example,

$$\boldsymbol{\phi}_3 = \phi_{30}\mathbf{i}_0 + \phi_{31}\mathbf{i}_1 + \phi_{32}\mathbf{i}_2 + \ldots + \phi_{3n}\mathbf{i}_n \qquad \ldots (13)$$

where the ϕs have been evaluated over the same set of points for which the hs were given, and in the same order. When expression (11) has been fitted, a series of calculated z values $z_0, z_1, \ldots, z_n$, can be obtained and these will likewise form the components of a vector $\mathbf{z}$ such that

$$\mathbf{z} = z_0\mathbf{i}_0 + z_1\mathbf{i}_1 + z_2\mathbf{i}_2 + \ldots + z_n\mathbf{i}_n. \qquad \ldots (14)$$

Thus $\mathbf{z}$, $\mathbf{h}$ and $\boldsymbol{\phi}$s may be regarded as vectors in an observation space of n dimensions. The $\boldsymbol{\phi}$ vectors may also be regarded as a set of vectors in function space which spans the 5-dimensional function subspace of this example, and so the expression may be written

$$\mathbf{z} = a_0\boldsymbol{\phi}_0 + a_1\boldsymbol{\phi}_1 + a_2\boldsymbol{\phi}_2 + a_3\boldsymbol{\phi}_3 + a_4\boldsymbol{\phi}_4 + a_5\boldsymbol{\phi}_5. \qquad \ldots (15)$$

If the disposable constants of (12) are now chosen in such a way that the scalar product of each $\boldsymbol{\phi}$ vector with another $\boldsymbol{\phi}$ vector is zero, i.e. if the $\boldsymbol{\phi}$ vectors are made orthogonal, then by the usual process of taking scalar products through (15) the coefficients are determined as

$$a_r = \frac{\mathbf{h} \cdot \boldsymbol{\phi}_r}{\phi_r^2}, \quad r = 0, 1, \ldots, 5. \qquad \ldots (16)$$

Thus the unknown coefficients are given directly by a series of independent equations, no determinants are involved, and the question of ill-conditioning does not arise. It may be shown that the coefficients found in this way are the same as those found by a direct derivation from the least-squares principle. This means that the restrictions of the traditional method have been removed and fitting by expressions of power much higher than that of a quadric becomes possible.

The process has been discussed so far in relation to a bivariate quadric fitting, but the extension to a higher number of variables is straightforward. Given any set of base variables such as

$$1, x, y, z, x^2, yx, y^2, zx, zy, z^2, \ldots, \qquad \ldots (17)$$

to take a trivariate case as an example, a set of orthogonal base functions $\phi_0, \phi_1, \phi_2, \ldots$ can be constructed by means of the Gram-Schmidt orthogonalization process.[10]

Let the base vectors corresponding to the base variables (17) be

$$\mathbf{1}, \mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{x}^2, \mathbf{yx}, \mathbf{y}^2, \mathbf{zx}, \mathbf{zy}, \mathbf{z}^2, \ldots, \qquad \ldots (18)$$

then a mutually orthogonal set of base vectors is given by

$$\left.\begin{aligned}
\boldsymbol{\phi}_0 &= \mathbf{1} \\
\boldsymbol{\phi}_1 &= \mathbf{x} - \frac{\boldsymbol{\phi}_0 \cdot \mathbf{x}}{\phi_0^2}\boldsymbol{\phi}_0 \\
\boldsymbol{\phi}_2 &= \mathbf{y} - \frac{\boldsymbol{\phi}_1 \cdot \mathbf{y}}{\phi_1^2}\boldsymbol{\phi}_1 - \frac{\boldsymbol{\phi}_0 \cdot \mathbf{y}}{\phi_0^2}\boldsymbol{\phi}_0 \\
\boldsymbol{\phi}_3 &= \mathbf{z} - \frac{\boldsymbol{\phi}_2 \cdot \mathbf{z}}{\phi_2^2}\boldsymbol{\phi}_2 - \frac{\boldsymbol{\phi}_1 \cdot \mathbf{z}}{\phi_1^2}\boldsymbol{\phi}_1 - \frac{\boldsymbol{\phi}_0 \cdot \mathbf{z}}{\phi_0^2}\boldsymbol{\phi}_0 \\
\boldsymbol{\phi}_4 &= \mathbf{x}^2 - \frac{\boldsymbol{\phi}_3 \cdot \mathbf{x}^2}{\phi_3^2}\boldsymbol{\phi}_3 - \frac{\boldsymbol{\phi}_2 \cdot \mathbf{x}^2}{\phi_2^2}\boldsymbol{\phi}_2 - \frac{\boldsymbol{\phi}_1 \cdot \mathbf{x}^2}{\phi_1^2}\boldsymbol{\phi}_1 - \frac{\boldsymbol{\phi}_0 \cdot \mathbf{x}^2}{\phi_0^2}\boldsymbol{\phi}_0
\end{aligned}\right\} \qquad \ldots (19)$$

and so on. This process can be applied to any original set of base vectors to produce an orthogonal set. If an orthonormal set is required then it is simply a matter of dividing by ϕ^2 at each stage. Thus the extension of the orthogonal fitting method to a higher number of dimensions than two becomes a matter of rote, and it should therefore be possible to extend the process to four dimensions to take care of the problem of fitting off-time and/or off-level reports from aircraft, merchant ships, and satellites.

Recurrence relationships

Although the Gram-Schmidt process may be used to orthogonalize a set of base vectors it will be noticed from (19) that the formation of each $\boldsymbol{\phi}$ requires the use of all the previously formed $\boldsymbol{\phi}$s. On a computer where the time factor is important this is a disadvantage, and some saving of effort may be achieved by using certain recurrence relationships amongst the ϕs. It was shown by Forsythe[4] that in the one-dimensional case the ϕs are represented by a relationship of the type

$$\phi_{n+1}=(x-c_n)\ \phi_n-c_{n-1}\ \phi_{n-1}\,. \qquad \ldots (20)$$

Cadwell and Williams[11] have shown that in two dimensions two similar relationships obtain and Weisfeld[12] has studied the higher-dimensional case. For more than two dimensions the computational procedures associated with the use of recurrence relationships become so complex as to make it doubtful whether this method has any great advantage over the Gram-Schmidt process. However, there is some evidence to show that recurrence relationships are always better behaved as regards the build-up of round-off errors.

The three stages of an orthogonal fitting technique

The underlying theory having been dealt with, the three stages of an orthogonal fitting may now be set down simply as:

(i) Calculate a sufficient set of orthogonal vectors.

(ii) Form the coefficients of the fitting function

$$a_r=\frac{\mathbf{h}\cdot\boldsymbol{\phi}_r}{\phi_r^2}\,.$$

(iii) Evaluate the fitting function over the required network of points.

It is instructive to consider the times taken for these three stages. In the ALGOL programme at present in use experimentally, the times for fitting a set of 132 observed heights by a 6th-power bivariate polynomial and evaluating over a network of 132 grid points are (for the three stages) approximately (i) 49 seconds (ii) 1·5 seconds (iii) 1·7 seconds. It is seen that the time for stage (i) is about 15 times greater than for (ii) and (iii) combined. Thus the actual fitting and evaluation is a computational triviality compared with the orthogonalization of the base vectors. This is a point of great significance in an application in which successive sets of observations are given at more or less the same set of base points because, as is evident from the foregoing theory, the orthogonal vectors are functions only of the base points, and they can therefore be computed once and for all, leaving only stages (ii) and (iii) to be gone through with each successive set of observations. With the saving of time that this entails the incentive to arrange the work to take advantage of this possibility is considerable. In the Meteorological Office's upper air analysis a major part of the problem is open to this possibility. Over oceanic

areas it would be necessary to take special steps to cover the likelihood of receiving ships' observations from non-standard positions. This might be done in a variety of ways, but two possibilities are worth mentioning here:

(*a*) A set of quasi-orthogonal vectors could be constructed over the field of possible position values. This would have the effect of making the matrix $\Phi\Phi$ a diagonally dominant type and the corresponding set of normal equations could then be swiftly solved by the Gauss-Seidel iteration.[2]

(*b*) A variation of the grid-point value correction technique described by Cressman[13] could be devised to provide a quick estimate of the field value at the standard position.

For the surface analysis where most of the ships would have variable positions it might be necessary to go through the whole routine and include stage (i), but even in this case it may still be possible to use either method (*a*) or (*b*). In this connection remarks made earlier (p. 3) concerning the unique position of the Office in the numerical engineering field with respect to accuracy are highly relevant here. Within the limits of the accuracy requirements, considerable liberties can be taken with computational routines to help overcome the problems of missing data, off-station weather ships and wrong or garbled observations, and every advantage must be taken of this fact to secure the possible saving of central processor time.

It is relevant here to mention the great versatility of the technique considered purely as a computational process. It can be put into different forms depending on the characteristics of the computer available. On COMET the ALGOL programme computes and stores the ϕ vectors successively through the storage area, so that in effect a matrix is stored row by row, and the vectors are accessed and used as required. However, this is a matter of computational expedience only. It is not essential, for the matrix stored is never handled as a matrix. All that ever happens is that the rows of the matrix are multiplied together component by component to form various scalar products. On COMET the relative speeds of arithmetic operations and accessing operations are such that it is significantly quicker to access a particular vector when it is wanted than to form it afresh each time by generating it from the corresponding ϕ polynomial. On some future machine it may well be that these relative speeds are such as to confer no advantage to storing and accessing. In this case it will be possible to do the whole process by means of a small compact programme using virtually no storage space, thus leaving the bulk of the machine's capacity available for other simultaneous use. The advantage of this is so great that it would seem desirable to make such a speed of arithmetic operation part of the specification for a future machine.

SOME ADVANTAGES ARISING FROM THE USE OF AN ORTHOGONAL TECHNIQUE

The main advantages of being able to fit to a higher power and in more dimensions have been adequately covered already, but there are a number of by no means negligible subsidiary benefits which may be obtained.

Quality control

At various stages of the process certain useful information of a statistical character is made available incidentally. For example, at any stage the residual sum of squares is given by

$$R_k^2 = (\mathbf{h} - a_0\phi_0 - a_1\phi_1 - \ldots - a_k\phi_k)^2 \qquad \ldots(21)$$

where ϕ_k represents the latest stage in the process. Now if at this stage some test is conducted and it is decided as a result to proceed one ϕ stage further, then the new residual sum of squares will be

$$R_{k+1}^2 = (\mathbf{h} - a_0\phi_0 - a_1\phi_1 - \ldots - a_k\phi_k - a_{k+1}\phi_{k+1})^2 \quad \ldots (22)$$

in which the coefficients $a_0, \ldots, a_k$ are precisely the same as those in (21); this is because a striking consequence of the orthogonality of the ϕs and the independence of the normal equations in the form (16) is that the computation of the next coefficient does not involve recomputing those already known. This is a point of particular contrast with the traditional method in which recalculation of all the coefficients previously found would have to take place.

An immediate consequence of (21) and (22) is that

$$R_k^2 - R_{k+1}^2 = a_{k+1}^2\phi_{k+1}^2, \quad \ldots (23)$$

which means that the contribution to the residual sum of squares of the individual term $a_{k+1}\phi_{k+1}$ is known. This is useful statistical information, as over a series of trials it may be found that certain ϕs contribute little to the process and can be omitted, thus shortening the calculations. Although the ALGOL programme has as yet had comparatively little use there is already indication that even-powered ϕs have more to contribute to the fitting than have odd-powered ϕs. It is surmised that the reason for this is that most synoptic patterns have a considerable measure of symmetry about them and therefore lend themselves more readily to description in terms of even-powered functions.

Although the question of the contribution of individual terms is important, a more immediate practical requirement will be to know the contribution made to the fitting by certain groups of terms such as those having a common total degree in x and y. This contribution is obviously known by the same argument as led to (23), and it is clearly possible to test whether sufficient variance has been extracted and if not to proceed to the next power level.

By a very trivial extension of the fitting computations the correlation index between the fitted surface and the original observations can be calculated, and in any extended routine use of such a programme a fairly firm estimate of the population of such indices could soon be reached. It would thus be possible to arrange for some type of alarm printing to alert the forecaster if the correlation index lay outside certain prescribed bounds either way. Alternatively if a line drawer with a pecked-line facility were being used the output could jump to pecked-line form in such an area, being full line elsewhere.

Apart from day-to-day quality control of output, such information is clearly exactly what is needed to determine the effect of those changes of procedure which inevitably have to be introduced from time to time as requirements change, and indeed as supposed improvements to the routine are thought of. At present it is extremely uncertain what the effect of such changes is, the quality control information being too scanty and too coarse to permit of any firm objective judgement.

Representation and storage of processed data

At present the analysed fields are known and stored as sets of 1927 values, a formidable problem of storage and access. In the proposed orthogonal process, after fitting has taken place the analysed data are then completely represented by the coefficients of the fitting function. These are considerably fewer in number than the individual grid points over which the fitting function may have to be evaluated. The exact ratio of coefficients to grid-point evaluations does of course depend upon the degree of fitting necessary and this in turn is a

matter of judgement, whether the judgement is exercised internally by some statistical control or whether it is exercised externally by a subjective human assessment. As a guide the case previously cited (p. 7) of fitting 132 observations and evaluating over 132 points may be considered. A 6th-power fitting will be found adequate for many purposes since in general it will provide, over this sort of area, an analysis a little superior to the analysis provided by the present analysis programmes. This involves 28 coefficients and thus the ratio of coefficients to processed data values is 7:33, say roughly 1:5. On the other hand, an 8th power involving 44 coefficients will, over the same sort of area, provide an analysis about as good as is likely to be drawn by a human analyst, at any rate under working conditions. This involves a ratio of coefficients to data values of 1:3. Either way it is a worth-while saving as the problem grows with time and with increasing commitments.

A basis for research

There are potentially profitable lines of research which may be thwarted by the present lack of quality in the differential fields of the present analyses. With a zero-order discontinuity between each grid-point value the present practice can make little claim to be an adequate representation of the differential geometry of a synoptic situation, and yet in some investigations a knowledge of the differential geometry is all-important. In this connection mention can be made of certain present investigations into the nature of clear-air turbulence and also a new development in the theory of fronts which depends heavily upon a detailed knowledge of high-order spatial derivatives.

There is also the point that a dependence on a finite-difference technology is no longer necessary, as derivatives can be obtained by differentiating the fitting function.

Provided problems connected with digitalization are overcome, the technique will provide a possible means of making a direct use of satellite information and other data connected directly with meteorological elements.

Constraint fitting

It is unlikely for many years to come that the human element will be entirely eliminated, though because of the relative slowness of human operations it will be desirable to keep them to the unavoidable minimum, at any rate in those parts of the schedule where speed of operation matters. The forecaster is able to draw upon a fund of experience which is very difficult to simulate in a machine, and in areas where data are sparse, or even absent altogether, it may be that the forecaster's opinion as to what is going on will be the best available assessment for a long while to come. It is desirable therefore that a future analysis system should provide a facility for intervention and that such intervention should be precise. With a high-powered fitting technique such precision is attainable. The coefficients in the fitting expression may be regarded as the number of degrees of freedom available to the process to enable it to account for the geometry of the surface. The greater the number of geometrical features on the surface the greater the number of degrees of freedom the fitting process requires and thus the greater will be the power of the fitting expression which adequately represents the surface.

If there is a limitation to quadric fitting, then there are only 6 degrees of freedom available and use of any on refinements to the technique cannot be afforded. They must all be used on the main problem. However, if something like an 8th-power bivariate expression having 44 degrees of freedom can be fitted then the possibility of using some of these for some special purposes is evident. Such a purpose is 'constraint fitting'.

Instead of fitting an expression like

$$z = a_0\phi_0 + a_1\phi_1 + a_2\phi_2 + \ldots + a_n\phi_n$$

i.e. $$z = \mathrm{f}(\phi),$$

consider instead the effect of fitting

$$z = H_1 + (x-b)\,\mathrm{f}(\phi) + (y-c)\,\mathrm{g}(\phi), \qquad \ldots (24)$$

where $\mathrm{g}(\phi)$ is another function of ϕ. A straightforward modification of the technique will enable this to be done and the result will be that at the point $x=b$, $y=c$ the fitted value must take up the mandatory value H_1. The fitting has been carried out according to least squares but subject to this constraint. No restriction has been placed upon the gradient at the point $x=b$, $y=c$, and so the point is not necessarily a centre; it may be a point on a slope.

Consider further the effect of fitting

$$z = H_1 + [(x-b)^2 + (y-c)^2]\,\mathrm{f}(\phi). \qquad \ldots (25)$$

Now not only does $z=H_1$ at $x=b$, $y=c$, but on differentiating by $\partial/\partial x$

$$\frac{\partial z}{\partial x} = 2(x-b)\mathrm{f}(\phi) + [(x-b)^2 + (y-c)^2]\,\mathrm{f}_x(\phi), \qquad \ldots (26)$$

and likewise

$$\frac{\partial z}{\partial y} = 2(y-c)\mathrm{f}(\phi) + [(x-b)^2 + (y-c)^2]\,\mathrm{f}_y(\phi); \qquad \ldots (27)$$

so that at the point (b, c), $z=H_1$ and $\nabla z=0$. This type of specification enables a centre to be fixed.

The process can be generalized by fitting

$$z = H_1 + \mathrm{g}(x, y)\mathrm{f}(\phi), \qquad \ldots (28)$$

whereupon the fitted field of values takes up any predetermined value either at a point or along some curve. Thus it would be possible for a forecaster in the future to specify the position of say the 528-decametre contour line in a given area of the analysis where no observations were available. Should it be deemed vital he could even specify precisely the sort of contour profile a particular low must have.

Another type of constraint fitting may arise in a region where the observations are heterogeneous as regards quality. It may be found desirable in such a region to arrange for a certain sub-set of observations to exert a dominating influence on the analysis. When four-dimensional fitting becomes an actuality, the North Atlantic would be an example of such a region. It may be that over a period of several hours the nine weather ships will be heavily outnumbered by aircraft, and it may be found desirable, after preliminary quality checks have been met, to fit the weather ships exactly whilst the aircraft are fitted with each other and with the weather ships according to the principle of least squares. With plentiful degrees of freedom available this too can be arranged. Mathematically the problem is that given N observations, n of them must be fitted exactly whilst the remaining $(N-n)$ must fit with each other and with the n according to least squares. The general non-orthogonal solution to this problem has been provided by Chew and Synge.[14] It is worth emphasizing again that this type of constraint fitting is only practicable if an adequate number of degrees of freedom are available.

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APPENDIX I

Some cases of actual fitting by high-powered polynomials are now presented. The first 11 diagrams illustrate the results of successively fitting a given synoptic pattern by bivariate polynomials of degrees 1 to 10.

Figure 1

This shows the actual chart situation at 300 mb on 6 March 1952 at 1500 GMT. The grid-point values were estimated and used as data for the fitting programme.

Note that the pattern has three main features:

(i) the low off north-west Scotland,
(ii) the ridge from the south, and
(iii) the col in the north-east,

and a minor feature is the weak trough over north-west France.

Figure 2

This fitting by a first-degree polynomial shows the best fitting plane.

Figure 3

This is a quadric fitting and the contours are conics. Even at this low power the beginning of the ridge from the south is evident, but with the small number of coefficients available in a quadric expression the function has not enough degrees of freedom to include any other feature.

Figure 4

Now, with 10 degrees of freedom, the 3rd-power function has got all the essential large-scale ingredients of the pattern, though it does not fit them very well.

Figure 5

Now the col in the north-east has become quite realistic and the low is beginning to take up its correct position, but note that with 15 degrees of freedom the 4th-power function has nothing to spare for the weak trough over north-west France.

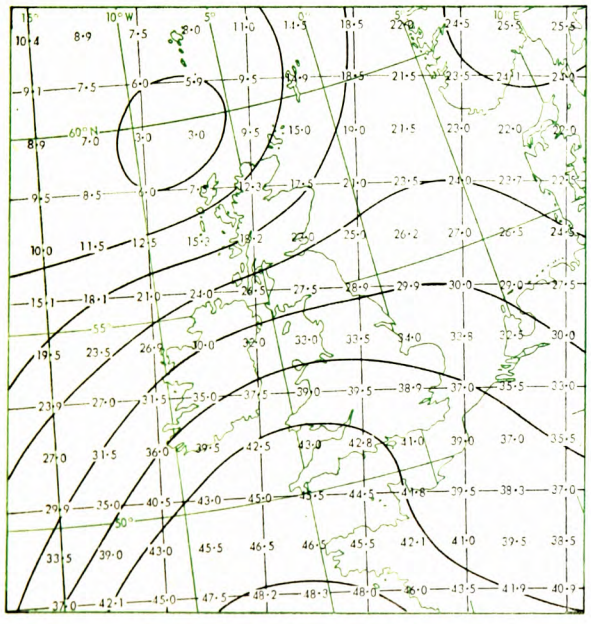

FIGURE 1. The original height field at 300 mb for 1500 GMT on 6 March 1952. Contours are at intervals of 6 decametres.

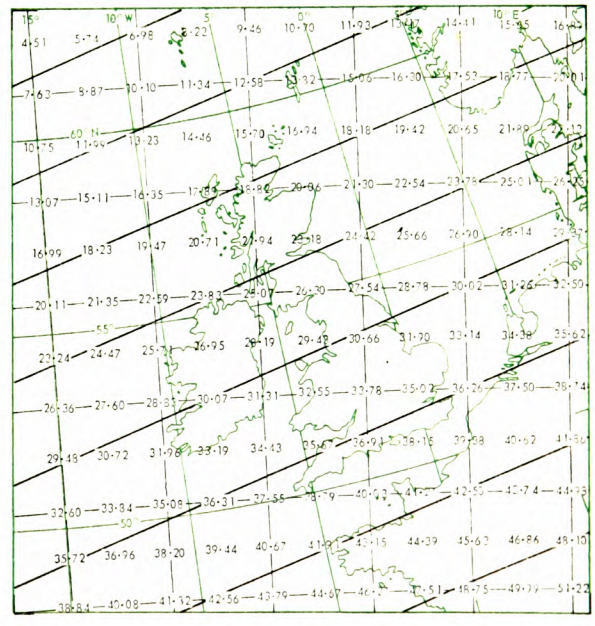

FIGURE 2. Surface fitted by $h=\phi(x, y)$ to 1st power.

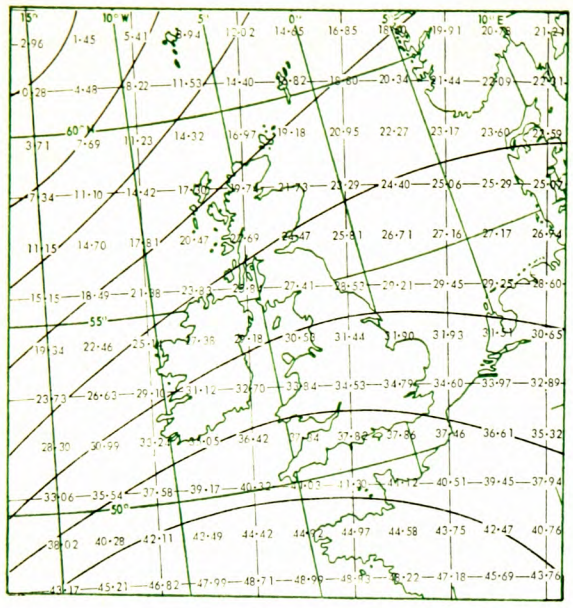

FIGURE 3. Surface fitted to 2nd power.

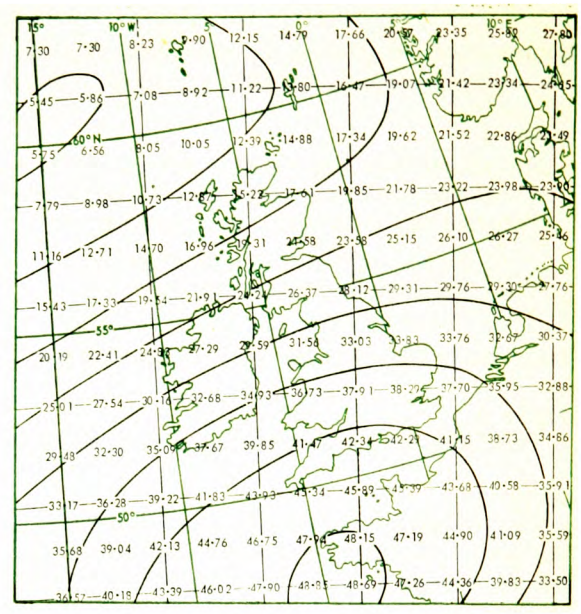

FIGURE 4. Surface fitted to 3rd power.

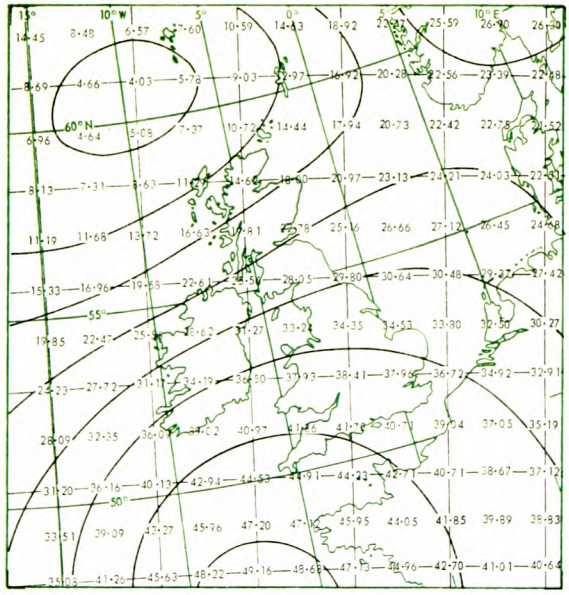

FIGURE 5. Surface fitted to 4th power.

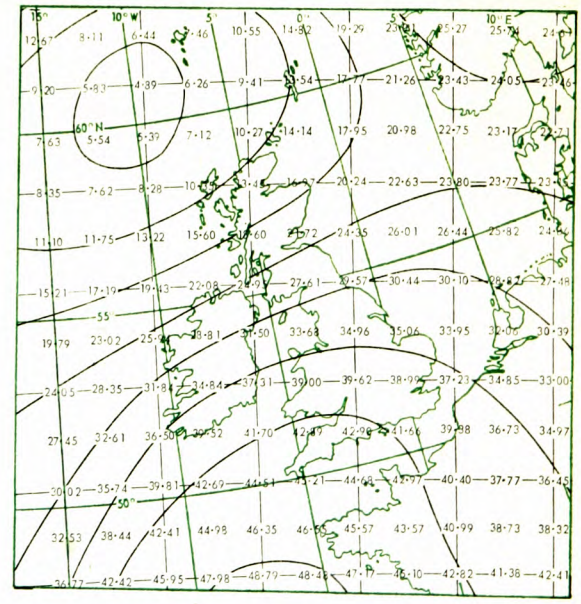

FIGURE 6. Surface fitted to 5th power.

Figure 6

At power 5 the whole pattern begins to look quite realistic and even the weak trough over France has begun to appear.

Figure 7

At the 6th power all the features listed for the original field are now quite well reproduced, and from this stage on it becomes impossible to judge the goodness of fit very well on the simple basis of a visual inspection

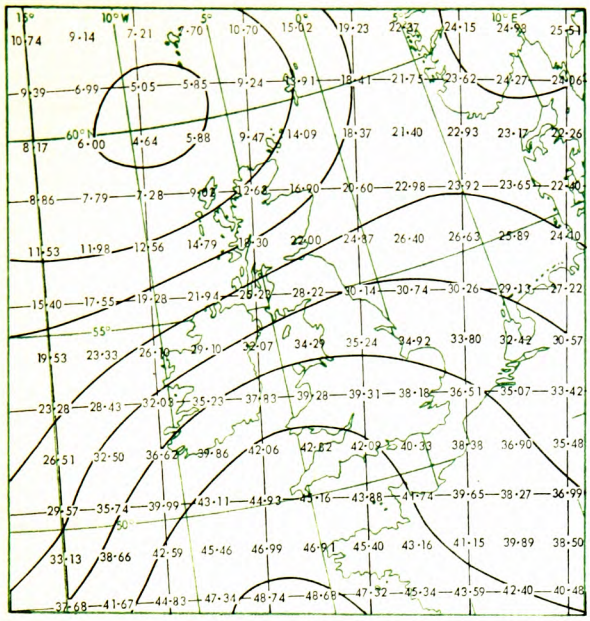

FIGURE 7. Surface fitted to 6th power.

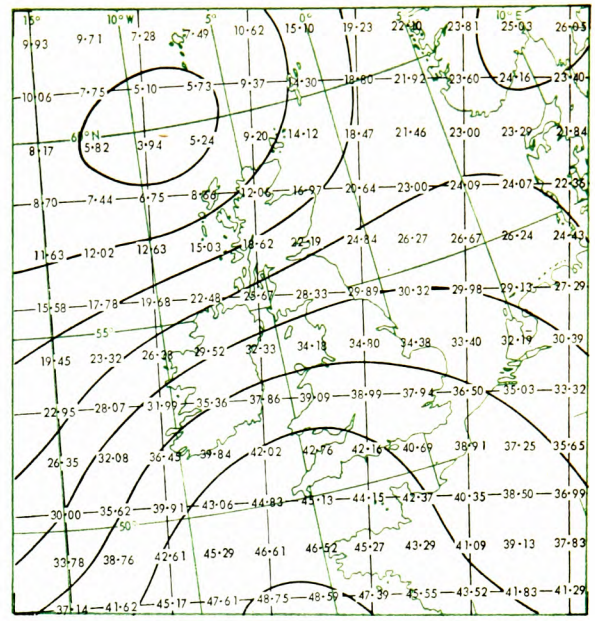

FIGURE 8. Surface fitted to 7th power.

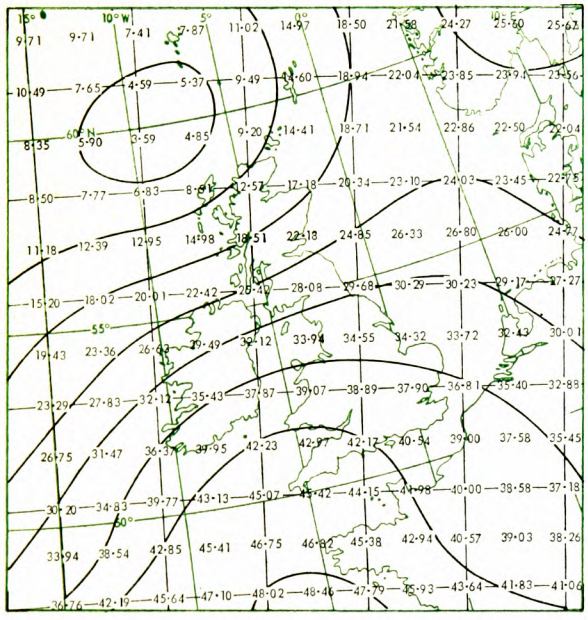

FIGURE 9. Surface fitted to 8th power.

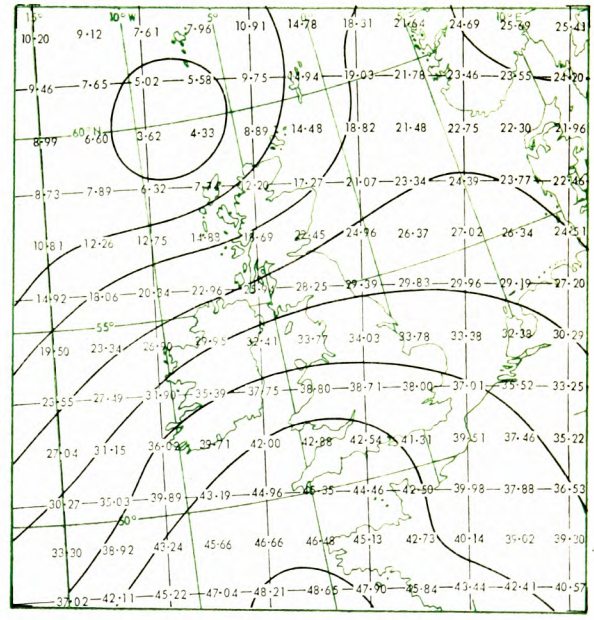

FIGURE 10. Surface fitted to 9th power.

of the global geometry. There is now the matter of considering how well the differential geometry is fitted and this is not done effectively by eye. It should be noted, however, that in the region of Stornoway (Scotland) the gradient is not correct.

Figure 8

The gradient over Stornoway is now reasonably correct.

Figures 9 *and* 10

Comparing these with Figure 7 it is noted that the gradient over Stornoway is much better and the central pressure of the low is more nearly correct.

Figure 11

Compare this with Figure 9 for the 8th-power fit. About all the eye can be sure of is that the central pressure of the low is still nearer to being correct. Other apparent differences are mainly concerned with the difference between one by-hand drawing and another. The real difference between Figures 9 and 11 lies in subtle differences in the differential geometry.

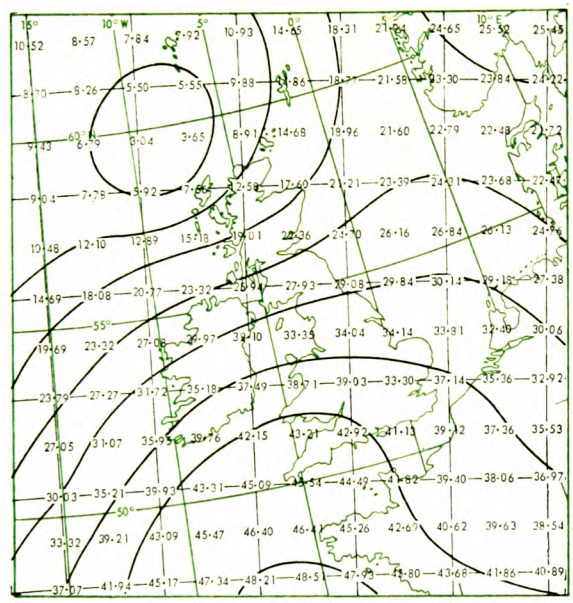

FIGURE 11. Surface fitted to 10th power.

APPENDIX II

The result of fitting an actual situation by means of high-powered polynomials is shown in Figures 12–15; the observations used are the same as those used by COMET to do the same analysis by the current grid-pointwise technique.

Figure 12 shows the 500-millibar analysis for 0000 GMT on 15 April 1968 which was hand-drawn in the Central Forecasting Office; this will be taken as a standard for the sake of comparisons. Note the synoptic features which provide the main points of comparison, namely the low near ocean weather station 'K', the trough near 'A', the trough over England and Wales, and the trough over the western Mediterranean. These are the features which need to be fitted well on the analysis.

Figure 13 shows the analysis produced by the grid-pointwise technique at present used in the Meteorological Office. This is quite a good representation, but the following defects are noticeable:

(i) The trough over England and Wales is too weakly represented.

(ii) The trough over the western Mediterranean does not have the right shape, the gradient over Elmas (Sardinia) being south-westerly instead of southerly.

(iii) The trough near station 'A' is a little displaced with the result that the height over 'A' is about 6 decametres too low.

(iv) Height has been lost over the eastern Mediterranean, particularly in the area south of Cyprus.

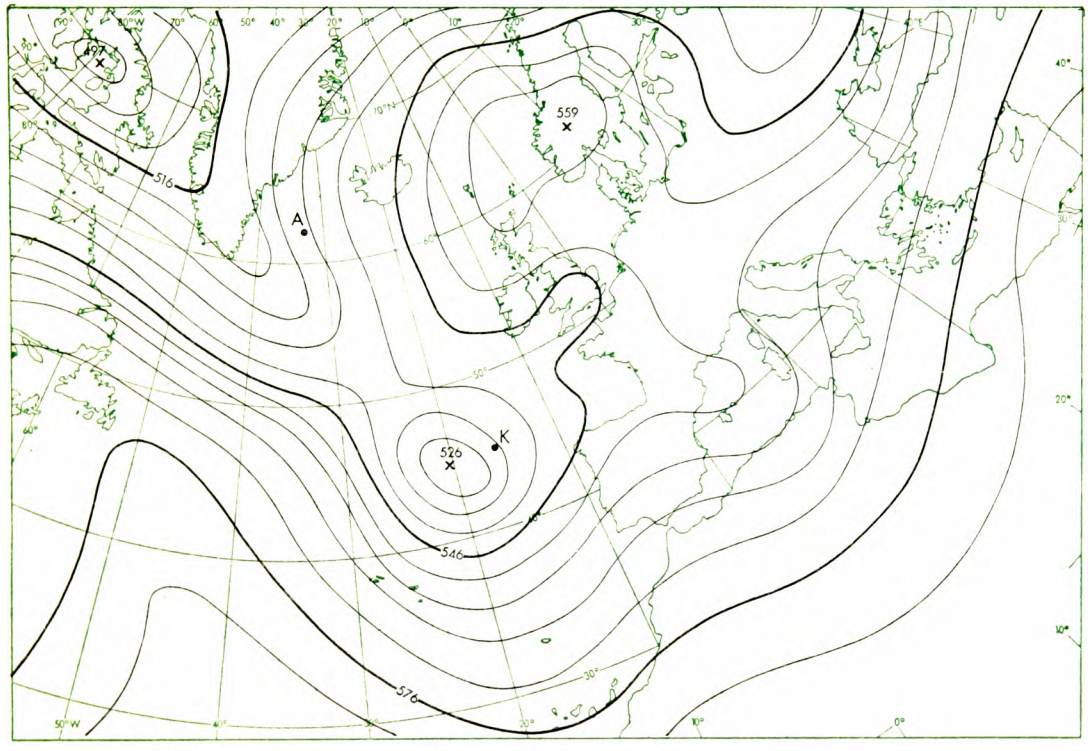

FIGURE 12. Contours at 500 mb for 0000 GMT on 15 April 1968 hand-drawn in the Central Forecasting Office.
Contours are at intervals of 6 decameters.

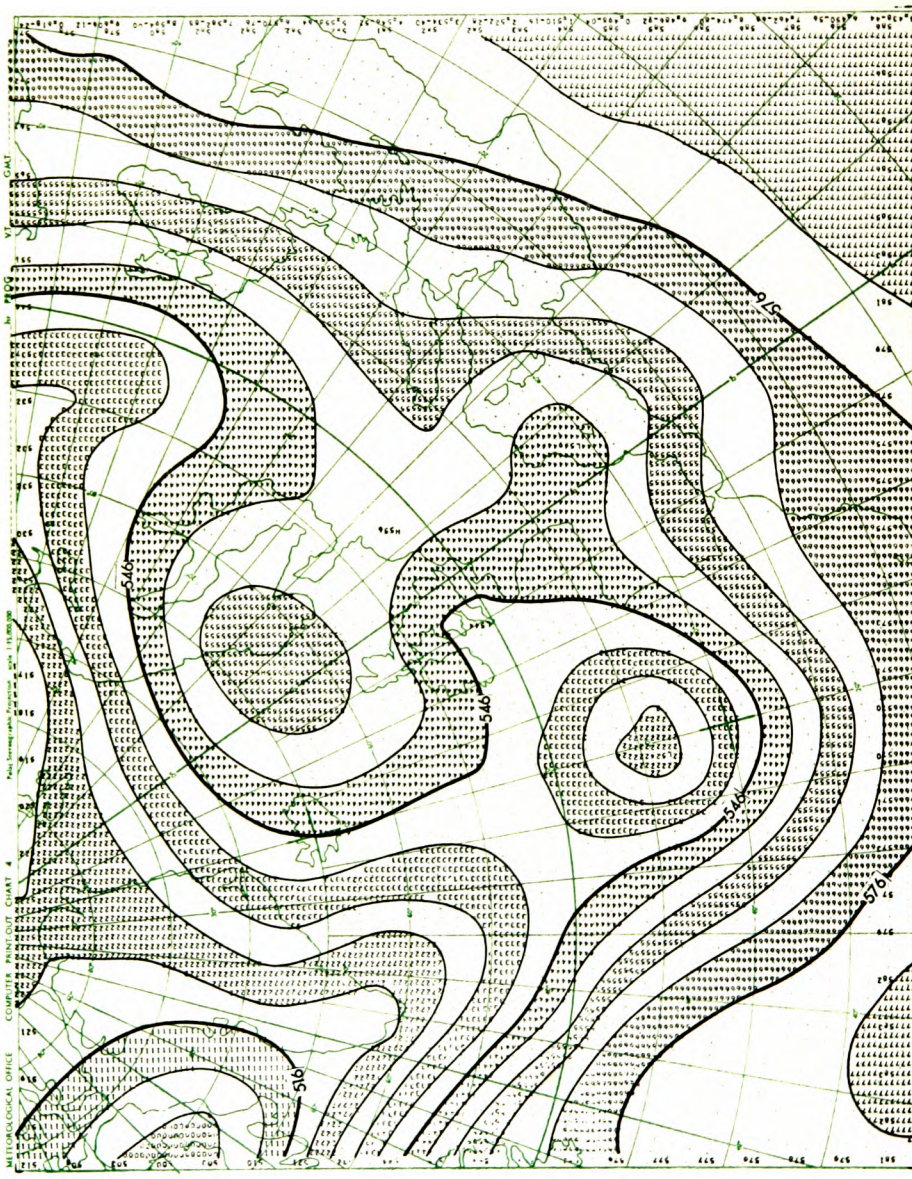

FIGURE 13. COMET analysis produced by the grid-pointwise technique.

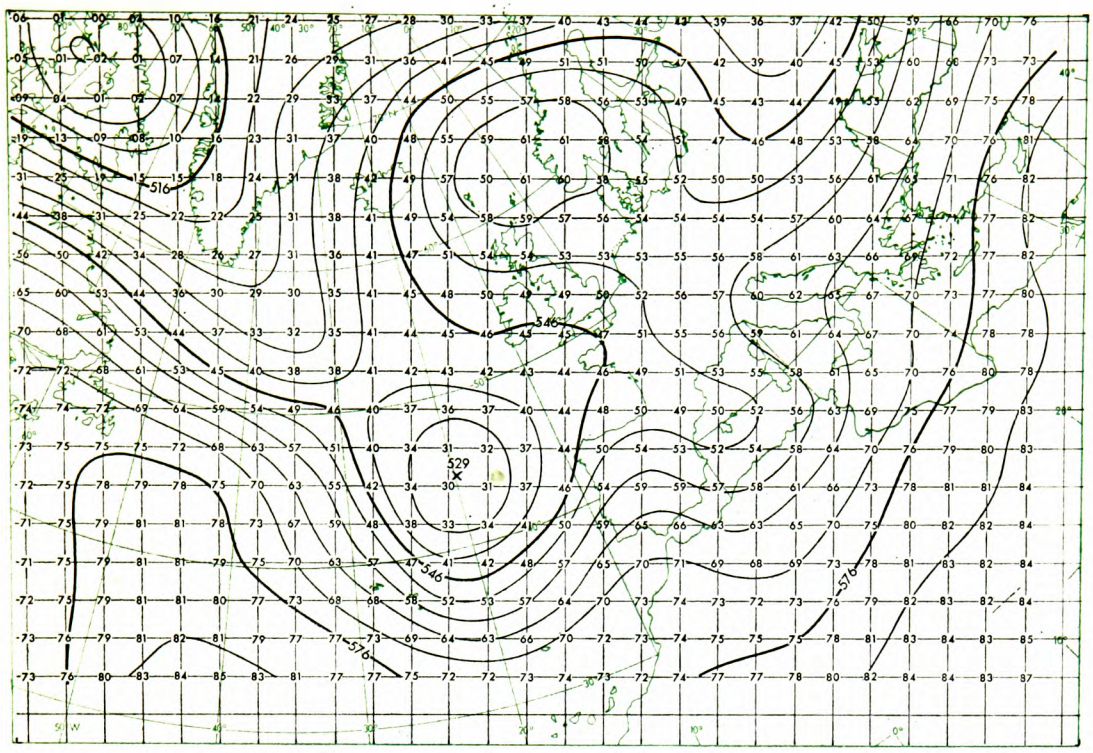

FIGURE 14. Analysis with surface fitted to 6th power (one sweep).

Figure 14 shows the result of fitting the area using six groups of overlapping observations fitted to the 6th power. In comparing Figure 14 with Figure 13 it must be kept in mind that Figure 13 is the result of a complete analysis process consisting of the following steps:

(i) A first sweep of grid-pointwise quadric fitting.

(ii) A second sweep of plane fitting to provide reference surfaces for checking the observations.

(iii) A third sweep in which the grid-point curvatures are calculated and the winds used are corrected for cyclostrophic effects.

(iv) A final sweep of fitting using the corrected winds and with faulty observations rejected.

On the other hand, Figure 14 is the result of only a single sweep of 6th-power fitting. Furthermore, although the same observations were used in both cases, for the 6th-power fitting no use was made of winds except over the sea areas. In particular no winds were used over the United Kingdom. It will be seen that the result of this single sweep of fitting compares quite well with the result of the full present technique. The low near station 'K' is slightly underfitted, but in other respects the 6th-power chart is as good as or perhaps slightly better than the one based on quadric fitting.

Figure 15 shows the result of fitting to the 8th-power. This time, winds over the U.K. have been used as well as those over the sea. Figure 15 is still the result of a single sweep of fitting, but even so it is clearly superior to that produced by the present method.

There are two main methods of utilizing winds in an analysis:

(1) It is possible to minimize an expression of the type

$$\sum(h-h_i)^2+T^2\sum_i(\mathbf{V}-\mathbf{V}_i)^2$$

where the h_i are the observed contour heights, the $\mathbf{V}_i$ are observed winds, and T decides the relative weight to be given to contour height and wind observations.

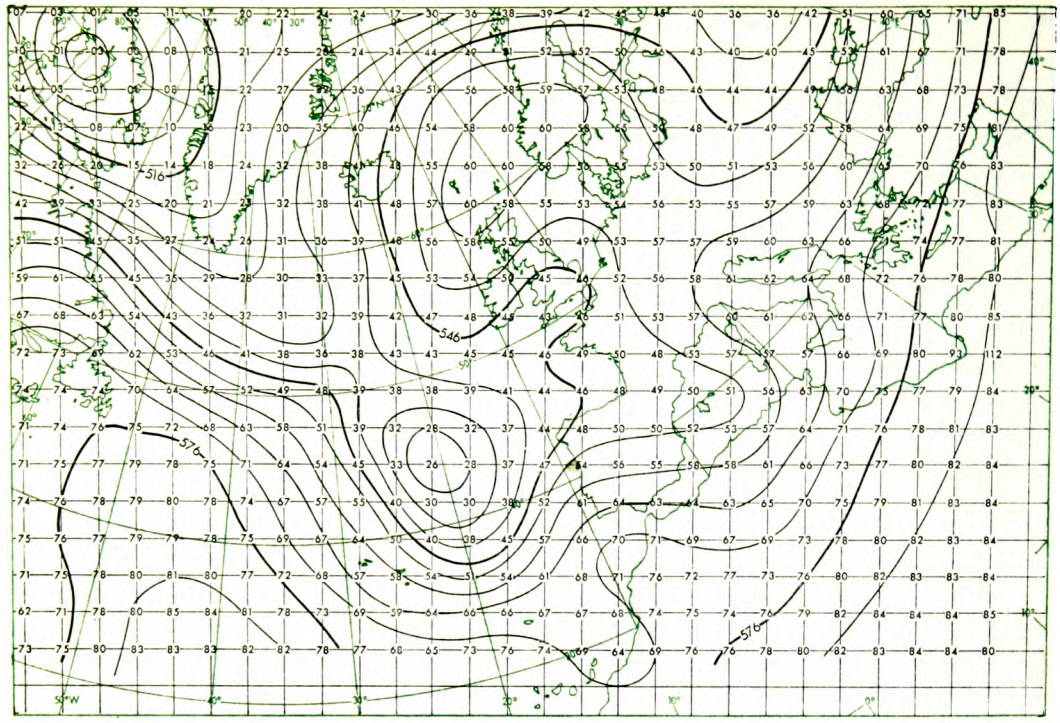

FIGURE 15. Analysis with surface fitted to 8th power (one sweep).

(2) It can be assumed that the geostrophic relationship between the contour field and the wind gives an adequate approximation to the slope of the pressure surface; this slope is then used to provide estimates of the contour height at some distance r away from the station in the x and y directions.

In method (1) T is arbitrary and the most suitable value must be determined by experiment. In method (2) r is arbitrary and must be found by experiment. Method (2) was used in the example described above and r was made equal to one grid length, but the optimum value for r has not yet been determined.

The problem of obtaining a smooth join at the edges of the six areas where they overlapped did not prove to be serious. A reasonable measure of preliminary agreement at the edges was ensured by allowing the groups of observations used to overlap somewhat. A further refinement was then obtained by allowing the actual computed grid points of each area to overlap by one row, the mean of the overlapping points being taken.

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